The Core Structure of the [001] Screw Dislocation in α-RDX

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Plastic deformation in crystalline solids is mediated by the formation and glide of crystal defects known as dislocations [1]. Dislocations are line defects that possess a long-range strain field that is described by linear elasticity and a core region around their elastic center where the displacements of atoms or molecules from their lattice sites are sufficiently large that inelastic relaxations take place. The atomic scale structure of the dislocation core, i.e., how the Burgers vector of the dislocation is distributed spatially into the crystallographic planes in the zone of the dislocation line, has a significant influence on the mobility of the dislocation and the planes on which it can glide [2].

The secondary explosive RDX (cyclotrimethylene trinitramine) is a molecular crystal that adopts an orthorhombic crystal structure in ambient conditions (α-polymorph) [3]. Despite its widespread use, a rigorous understanding of the mechanisms through which it deforms plastically has yet to be developed. Indentation studies have demonstrated that the primary slip system involves dislocations with Burgers vector [001] that glide on the (010) plane [4].

Atomistic studies of the core structure of the [001] screw dislocation in RDX have been performed in order to identify the slip planes in this material. Interatomic and intermolecular bonding in RDX is described using the non-reactive potential developed by Smith and Bharadwaj [5]. The simulation cell consisted of a cylinder three-Burgers-vectors thick and of diameter 460 Å. The axis of the cylinder was parallel to [001] and periodic boundary conditions were applied in this direction. A perfect screw dislocation (**b** = [001]) was introduced into the center of the block by applying to the centers of mass of all molecules the displacement field calculated using the anisotropic elastic theory of dislocations [1,6]. The elastic constants used in the anisotropic elasticity calculations were determined at 300K from the Smith potential. The equilibrium structure of the dislocation at 300K was determined by performing molecular dynamics simulations while keeping all atoms in the outer 30 Å of the block fixed at their initial positions.

The core structure of the [001] screw dislocation is represented by a differential displacement map in Fig. 1. In this figure, relative displacements of the molecular centers of mass parallel to the dislocation line, i.e., the screw component of the Burgers vector, are plotted. It is evident that the displacements are confined to the (010) plane and that the core is planar. This result is in excellent agreement with experiment since such a configuration strongly implies that the glide of [001] dislocations on (010) planes will have the lowest attainable Peierls stress, i.e., the primary slip planes are (010). The edge components of the Burgers vector were found to be extremely small and there is no indication that the dislocation dissociates into partials. Atomistic calculations of the Peierls stress for the glide of the [001] screw dislocation in α-RDX on (010), are currently underway in order to further resolve the experimental results in [4].

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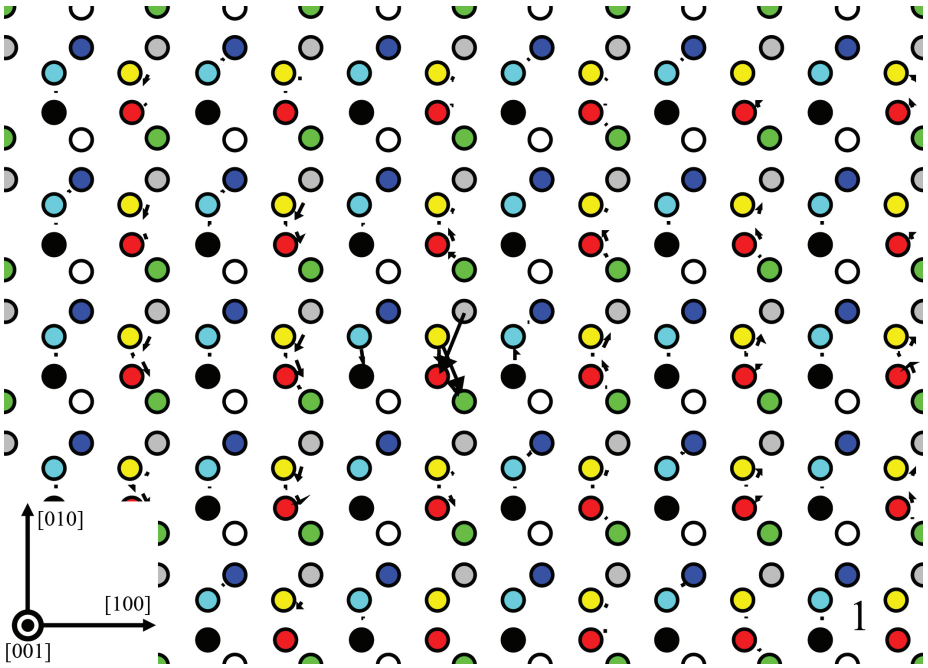

Fig. 1.
A differential displacement map of the core of the [001] screw dislocation in α-RDX. This map shows a projection perpendicular to the direction of the dislocation line, [001], of the centers of mass of molecules in one period of crystal. The colors differentiate molecular planes. The arrows represent relative displacements of centers of mass between neighboring molecules parallel to the dislocation line and their length is normalized such that it is equal to |b|/2.